



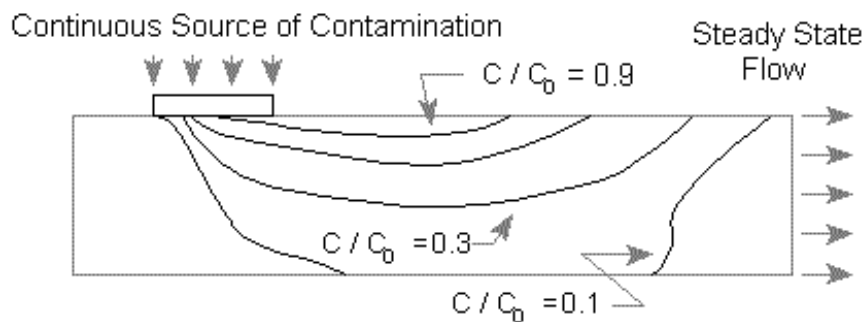
UNDERSTANDING VARIATION IN PARTITION COEFFICIENT, K_d , VALUES



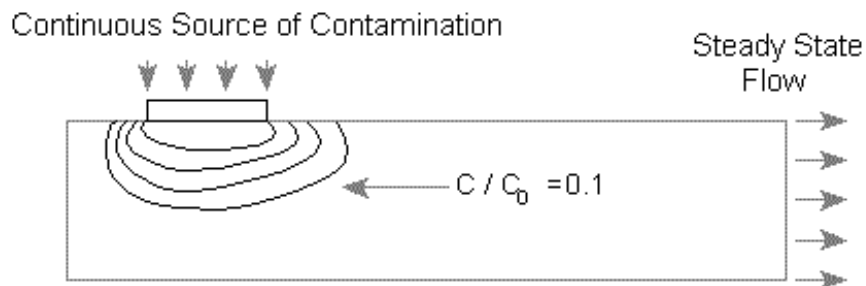
Volume I:

The K_d Model, Methods of Measurement, and Application of Chemical Reaction Codes

Case I: $K_d = 1$ ml/g



Case II: $K_d = 10$ ml/g



UNDERSTANDING VARIATION IN PARTITION COEFFICIENT, K_d , VALUES

Volume I:

**The K_d Model, Methods of Measurement, and
Application of Chemical Reaction Codes**

August 1999

A Cooperative Effort By:

**Office of Radiation and Indoor Air
Office of Solid Waste and Emergency Response
U.S. Environmental Protection Agency
Washington, DC 20460**

**Office of Environmental Restoration
U.S. Department of Energy
Washington, DC 20585**

NOTICE

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FOREWORD

Understanding the long-term behavior of contaminants in the subsurface is becoming increasingly more important as the nation addresses groundwater contamination. Groundwater contamination is a national concern as about 50 percent of the United States population receives its drinking water from groundwater. It is the goal of the Environmental Protection Agency (EPA) to prevent adverse effects to human health and the environment and to protect the environmental integrity of the nation's groundwater.

Once groundwater is contaminated, it is important to understand how the contaminant moves in the subsurface environment. Proper understanding of the contaminant fate and transport is necessary in order to characterize the risks associated with the contamination and to develop, when necessary, emergency or remedial action plans. The parameter known as the partition (or distribution) coefficient (K_d) is one of the most important parameters used in estimating the migration potential of contaminants present in aqueous solutions in contact with surface, subsurface and suspended solids.

This two-volume report describes: (1) the conceptualization, measurement, and use of the partition coefficient parameter; and (2) the geochemical aqueous solution and sorbent properties that are most important in controlling adsorption/retardation behavior of selected contaminants. Volume I of this document focuses on providing EPA and other environmental remediation professionals with a reasoned and documented discussion of the major issues related to the selection and measurement of the partition coefficient for a select group of contaminants. The selected contaminants investigated in this two-volume document include: chromium, cadmium, cesium, lead, plutonium, radon, strontium, thorium, tritium (^3H), and uranium. This two-volume report also addresses a void that has existed on this subject in both this Agency and in the user community.

It is important to note that soil scientists and geochemists knowledgeable of sorption processes in natural environments have long known that generic or default partition coefficient values found in the literature can result in significant errors when used to predict the absolute impacts of contaminant migration or site-remediation options. Accordingly, one of the major recommendations of this report is that for site-specific calculations, partition coefficient values measured at site-specific conditions are absolutely essential.

For those cases when the partition coefficient parameter is not or cannot be measured, Volume II of this document: (1) provides a "thumb-nail sketch" of the key geochemical processes affecting the sorption of the selected contaminants; (2) provides references to related key experimental and review articles for further reading; (3) identifies the important aqueous- and solid-phase parameters controlling the sorption of these contaminants in the subsurface environment under oxidizing conditions; and (4) identifies, when possible, minimum and maximum conservative partition coefficient values for each contaminant as a function of the key geochemical processes affecting their sorption.

This publication is the result of a cooperative effort between the EPA Office of Radiation and Indoor Air, Office of Solid Waste and Emergency Response, and the Department of Energy Office of Environmental Restoration (EM-40). In addition, this publication is produced as part of ORIA's long-term strategic plan to assist in the remediation of contaminated sites. It is published and made available to assist all environmental remediation professionals in the cleanup of groundwater sources all over the United States.

Stephen D. Page, Director
Office of Radiation and Indoor Air

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**TO COMMENT ON THIS GUIDE OR PROVIDE INFORMATION FOR FUTURE
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ABSTRACT

This two-volume report describes the conceptualization, measurement, and use of the partition (or distribution) coefficient, K_d , parameter, and the geochemical aqueous solution and sorbent properties that are most important in controlling adsorption/retardation behavior of selected contaminants. The report is provided for technical staff from EPA and other organizations who are responsible for prioritizing site remediation and waste management decisions. Volume I discusses the technical issues associated with the measurement of K_d values and its use in formulating the retardation factor, R_f . The K_d concept and methods for measurement of K_d values are discussed in detail in Volume I. Particular attention is directed at providing an understanding of: (1) the use of K_d values in formulating R_f , (2) the difference between the original thermodynamic K_d parameter derived from ion-exchange literature and its “empiricized” use in contaminant transport codes, and (3) the explicit and implicit assumptions underlying the use of the K_d parameter in contaminant transport codes. A conceptual overview of chemical reaction models and their use in addressing technical defensibility issues associated with data from K_d studies is presented. The capabilities of EPA’s geochemical reaction model MINTEQA2 and its different conceptual adsorption models are also reviewed. Volume II provides a “thumb-nail sketch” of the key geochemical processes affecting the sorption of selected inorganic contaminants, and a summary of K_d values given in the literature for these contaminants under oxidizing conditions. The contaminants chosen for the first phase of this project include chromium, cadmium, cesium, lead, plutonium, radon, strontium, thorium, tritium (^3H), and uranium. Important aqueous speciation, (co)precipitation/dissolution, and adsorption reactions are discussed for each contaminant. References to related key experimental and review articles for further reading are also listed.

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